

Pair Density Wave correlations in the Kondo-Heisenberg Model

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We show, using density matrix renormalization group calculations complemented by field theoretic arguments, that the spin gapped phase of the one dimensional Kondo-Heisenberg model exhibits quasi-long range superconducting correlations *only* at a non-zero momentum. The local correlations in this phase resemble those of the pair density wave state which was recently proposed to describe the phenomenology of the striped ordered high temperature superconductor $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, in which the spin, charge, and superconducting orders are strongly intertwined.

Recent experiments in the high temperature superconductor $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ near doping $x = 1/8$ have revealed a dramatic layer decoupling effect in which anomalous mesoscopic 2D superconductivity persists well above the macroscopic 3D superconducting transition temperature, T_c . [1–3] Moreover, the superconductivity coexists with static stripe (charge and spin) order. It has been proposed that the anomalous superconducting properties are evidence of the existence of a novel type of superconducting state, the pair-density wave (PDW). [4–6]

The PDW is a state in which charge, spin and superconducting (SC) orders are *intertwined* in a spatially modulated fashion. The SC order has a wave vector \mathbf{Q} which is the same as that of the spin density wave (SDW) and half of the ordering wave vector $2\mathbf{Q}$ of the charge density wave (CDW). Its SC order is Larkin-Ovchinnikov-like, but without the magnetization of the latter. Although much is known about the properties of this state[5, 6], there is, as yet, no fully satisfactory microscopic theory.

In the context of Bardeen-Cooper-Schrieffer type mean-field theories, a PDW is only ever stable at strong coupling[7] (*i.e.* outside the regime in which such treatments are reliable). Slave-boson mean-field theories of the $t - J$ model find that, although the PDW is quite competitive energetically, it (barely) loses to the uniform d-wave SC state[8]. While early numerical variational Monte Carlo studies of the $t - J$ model found a regime in which the PDW appeared to be stable[9], more recent studies have found that it has slightly higher variational energy than the uniform d-wave state[10, 11].

In the present paper we study the superconducting correlations in the 1D Kondo-Heisenberg model (KHM). This is the simplest model in which one can investigate the interplay between strong antiferromagnetic ordering tendencies, represented by a Heisenberg chain, and possible superconducting and charge-density wave orders, derived from an itinerant electron band to which it is coupled. The 1D character of the model permits us to employ the powerful numerical density-matrix renormalization group (DMRG)[12] and analytic bosonization methods to solve the problem, despite the strong interactions.

On the down side, there are special features of 1D physics, which may raise questions concerning the applicability of the results to higher dimensional situations. On the other hand, especially since the order we are investigating is unidirectional, and thus has an essentially 1D geometry, it is plausible that the local structure of the correlations up to intermediate scales are dimension independent.

The key finding from our DMRG studies is that, for the range of parameters considered here, the 1D KHM exhibits a spin-gapped phase with quasi-long range (power-law) PDW correlations,*i.e.* superconducting correlations which oscillate with a period $2b$ where b is the lattice constant of the Heisenberg chain. At the same time the uniform singlet superconducting correlations are small and apparently fall exponentially with distance. Since the same model exhibits substantial, although short-ranged correlated, antiferromagnetic tendencies with the same period, this state can clearly be identified as a fluctuating version of the long-sought PDW. Note that the occurrence of a spin-gap in the 1D Kondo-Heisenberg model has been discussed insightfully in the literature[13, 14] and the possibility of an oscillatory superconducting order parameter was previously inferred on the basis of bosonization studies.[15–20] However, we believe that this is the first place in which the existence and character of this state has been derived from a microscopic model, and the nature of the correlations is elucidated.[21]

Model: The 1D KHM is defined as a one dimensional electron gas (1DEG) coupled to a spin- $\frac{1}{2}$ chain:

$$H = H_{\text{1DEG}} + H_{\text{Heis}} + H_K \quad (1)$$

where

$$H_{\text{1DEG}} = -t \sum_{j,\sigma} c_{j\sigma}^\dagger c_{j+1\sigma} + \text{h.c.} - \mu \sum_{j,\sigma} n_j, \quad (2)$$

$$H_{\text{Heis}} = J_H \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \quad (3)$$

$$H_K = J_K \sum_{j,a} S_j^a \left[c_{j\sigma}^\dagger (s^a)_{\sigma\sigma'} c_{j\sigma'} \right]. \quad (4)$$

Here, $c_{j\sigma}^\dagger$ creates an electron with spin σ at site j , \mathbf{S}_j is the spin $\frac{1}{2}$ operator of the spin chain, and $s^a = \frac{1}{2}\tau^a$

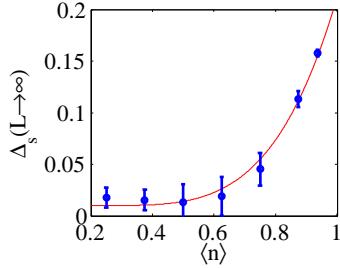


FIG. 1: (Color online.) The spin gap vs. the electron concentration in the 1DEG. $J_H = J_K = 2t$. The error bars are a result of the extrapolation to the thermodynamic limit. (Relative to the extrapolation error, the DMRG truncation error is negligible.)

($\tau^{a=x,y,z}$ are Pauli matrices).

In typical physical circumstances in which Kondo physics arises, one would expect J_H and $J_K \ll t$. In this limit, the length scales characterizing the Kondo effect are exponentially large, and hence not readily accessible by any numerical method. We therefore use $J_H \sim J_K \sim t$. On the basis of the field-theoretic analysis (see below), we expect the character of the phases to survives to small J/t . Moreover, the $J_H \sim J_K \sim t$ regime is not necessarily unphysical; it can be derived from the $U \rightarrow \infty$ limit of a Hubbard model on the spin-chain, with chemical potential chosen so that there is one electron per site, and with hopping matrix element along the chain, $t_H = \sqrt{J_H U}/2$, and hopping between the spin-chain and the 1DEG, $t_K = \sqrt{J_K U}/2$.

Numerical results: The model (1) was solved using DMRG on finite lattices with $L = 32 - 128$ and open boundary conditions. Up to $m = 1800$ states were kept, giving DMRG truncation errors smaller than 10^{-6} .

Fig. 1 shows the spin gap $\Delta_s = E_0(1) - E_0(0)$, where $E_0(S_z)$ is the ground state energy of a system with a z spin projection S_z . The spin gap was extrapolated to the thermodynamic ($L \rightarrow \infty$) limit. The results are shown for $J_H = J_K = 2t$, as a function of the concentration of electrons in the 1DEG, n . Due to the particle-hole symmetry of the model, it is sufficient to consider $n < 1$.

Near $n = 1$ there is a sizable spin gap[14]; Δ_s decreases away from $n = 1$. For $n = 1$ (not shown), the spin gap is $\Delta_s \approx 0.8$, but there is also a finite charge gap in the $L \rightarrow \infty$ limit. We henceforth focus on $n = 0.875$, for which Δ_s is substantial. Since Δ_s persists at lower densities, we expect the low-energy properties at smaller n to be similar, although the correlation length is larger.

PDW correlations: The opening of a spin gap is expected to lead to enhanced SC (as well as CDW) correlations. To study these correlations, we have applied a local pair field to the left boundary[22]:

$$H_{\text{pair}} = \Delta(c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger) + \text{h.c.} \quad (5)$$

where we fixed $\Delta = 0.5t$. (We have checked explicitly that the results do not depend on the size of Δ .)

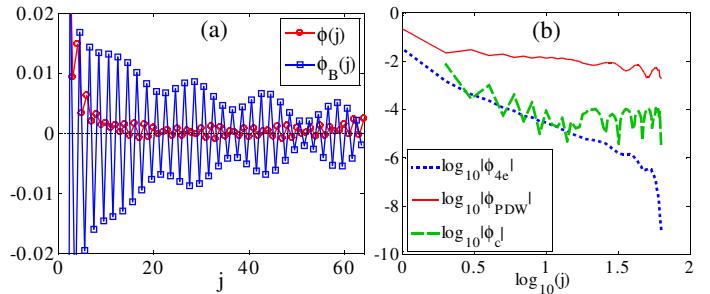


FIG. 2: (Color online.) (a) The SC order parameters ϕ and ϕ_B (see text) as a function of position in an $L = 64$ system with $n = 0.875$. (b) Measurements of ϕ_{PDW} , ϕ_{4e} , ϕ_c vs. position. The oscillatory behavior close to the right boundary is an edge effect.

The superconducting response of the system was probed by measuring the following induced order parameters throughout the system[23]:

$$\phi(j) = \langle c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle, \quad \phi_B(j) = \frac{1}{2} \langle c_{j\uparrow}^\dagger c_{j+1\downarrow}^\dagger - c_{j\downarrow}^\dagger c_{j+1\uparrow}^\dagger \rangle, \quad (6)$$

where $\phi(j)$ and $\phi_B(j)$ are, respectively, the expectation of the singlet pair creation operator on site j and on the bond from site j to site $j + 1$. Fig. 2a shows $\phi(j)$ and $\phi_B(j)$ in an $L = 64$ system. $\phi(j)$ appears to decay very rapidly away from the left boundary. $\phi_B(j)$ decays much more slowly, and exhibits pronounced oscillations as a function of position with wavevector $q = \pi/b$, as it changes its sign between every consecutive bonds. Longer periods are also apparent in the figure. These oscillations clearly indicate that the dominant pairing correlations are at a non-zero momentum.

Refs. [15–17, 19, 20] proposed, based on bosonization, that the spin-gapped phase of the KHM has dominant pairing correlations at a non-zero wavevector, described by a “composite” order parameter[20]

$$\phi_c(j) = (-1)^j \langle \left[\sum_{\sigma, \sigma'} c_{j-1\sigma}^\dagger (is^y \mathbf{s})_{\sigma\sigma'} c_{j+1\sigma'}^\dagger \right] \cdot \mathbf{S}_j \rangle. \quad (7)$$

In addition, PDW order should be accompanied by a uniform ($q = 0$) “charge 4e” order parameter[24]:

$$\phi_{4e}(j) = \langle c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger c_{j+1\uparrow}^\dagger c_{j+1\downarrow}^\dagger \rangle. \quad (8)$$

Fig 2b shows $\phi_{\text{PDW}}(j) \equiv (-1)^j \phi_B(j)$, as well as $\phi_c(j)$ and $\phi_{4e}(j)$, as a function of position, on a logarithmic scale. The largest, and most slowly decaying, order parameter is $\phi_{\text{PDW}}(j)$, suggesting that the system is best described as a fluctuating PDW state. As expected, $\phi_{4e}(j)$ and $\phi_c(j)$ are non-zero, but small. $\phi_c(j)$ is modulated as a function of position, while $\phi_{4e}(j)$ is smooth.

The wavevectors of the leading SC and CDW fluctuations can be determined by a Fourier analysis of the SC and CDW orders.[25] Fig. 3 shows the absolute values of

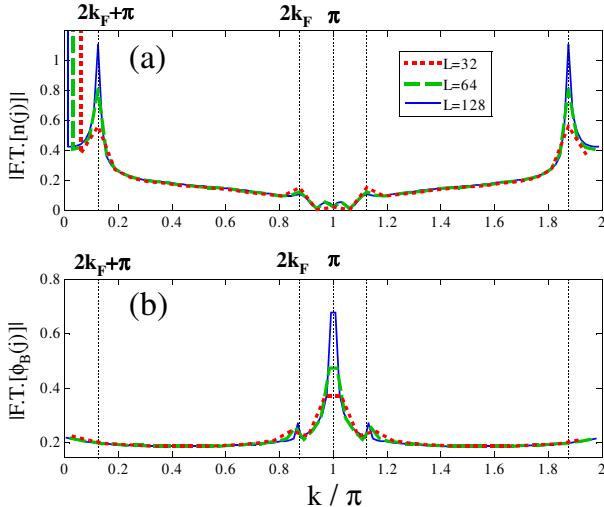


FIG. 3: (Color online.) Absolute values of the Fourier transforms of (a) the charge [$\langle n(j) \rangle$] and (b) the SC [$\phi_B(j)$] orders. $L = 32\text{--}128$.

the Fourier transforms of $\phi_B(j)$ and $n(j) \equiv \sum_{\sigma} c_{j\sigma}^{\dagger} c_{j\sigma}$ for system sizes between $L = 32$ and 128 . The charge density exhibits a large peak at $q = 2k_F + \pi/b$ which grows as a function of system size, where $2k_F \equiv \pi n$. There are also small sub-leading features at $q = 2k_F$ and $q = \pi/b$. The main feature in the Fourier transform of ϕ_B is a pronounced peak at $q = \pi/b$, with a sub-leading peak at $q = 2k_F$. This shows unambiguously that the dominant order in this system is a PDW with $q = \pi/b$, accompanied by CDW correlations at $q = 2k_F + \pi/b$.

In order to elucidate further the nature of the microscopic correlations in the system, we perform another simulation in which both a pair field [Eq (5)] and a Zeeman field, $H_Z = -hS_{j=1}^z$ ($h = 0.5t$) are applied to the left boundary of the system. The induced charge, superconducting, and magnetic ($\langle S_j^z \rangle$) order parameters are shown near the middle of the $L = 64$ system in Fig. 4a. The magnetic order oscillates at wavevector $q = \pi/b$ (the same as the PDW) with an envelope that decays exponentially on longer length scales.

Next, we would like to understand what determines the PDW wavevector. We performed another calculation in which the spin chain is “diluted”, *i.e.* there is one spin site for every *two* 1DEG sites. Eq. (3) is replaced by $\tilde{H}_{\text{Heis}} = J_H \sum_j \mathbf{S}_{2j} \cdot \mathbf{S}_{2j+2}$, and similarly $\tilde{H}_K = J_K \sum_{j,a} S_{2j}^a [c_{2j\sigma}^{\dagger} (s^a)_{\sigma\sigma'} c_{2j\sigma'}]$. Fig. 4b illustrates the results for $\langle S_j^z \rangle$, $\langle n_j \rangle$, and ϕ_B near the middle of an $L = 128$ system. (In order to maintain a large spin gap, n was taken to be 0.625.) Clearly, the PDW order changes sign across every spin site, indicating that the dominant PDW wavevector is again $q = \pi/b$, where now $b = 2$. Thus, the period of the PDW is tied to that of the local (fluctuating) magnetic ordering. The local correlations in Fig. 4a-b are a one dimensional version of the phenomenologically proposed “striped-superconducting”

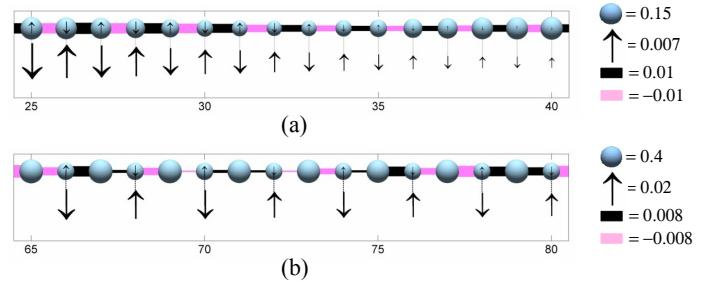


FIG. 4: (Color online.) Order parameters in (a) an $L = 64$ KHM chain with $n = 0.875$, and (b) an $L = 128$ “diluted” KHM chain (with one spin site for each two 1DEG sites) with $n = 0.625$. Circles: 1DEG hole density ($1 - \langle n(j) \rangle$), bond color/thickness: the bond-centered SC amplitude $\phi_B(j)$. The arrows show the spin density ($S^z(j)$).

state for $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$ [4].

Continuum limit: Analytical progress can be made in the limit $J_H, t \gg J_K$, where we may first take the continuum limit of both the 1DEG and the spin chain. We use a description in terms of the Bosonic fields φ_c, φ_s and $\tilde{\varphi}_s$, representing charge/spin fluctuations in the 1DEG and spin chain, respectively [and the respective conjugate fields θ_c, θ_s and $\tilde{\theta}_s$]. The Hamiltonian densities of the 1DEG and the spin chain take the form [13, 19, 20]

$$\begin{aligned} \mathcal{H}_{\text{1DEG}} &= \sum_{\alpha=c,s} v_{\alpha} \left[\frac{K_{\alpha}}{2} (\partial_x \theta_{\alpha})^2 + \frac{1}{2K_{\alpha}} (\partial_x \varphi_{\alpha})^2 \right] \\ \mathcal{H}_{\text{Heis}} &= \frac{1}{2} \tilde{v}_s [(\partial_x \tilde{\theta}_s)^2 + (\partial_x \tilde{\varphi}_s)^2] \end{aligned} \quad (9)$$

where K_c, K_s, v_c, v_s and \tilde{v}_s are, respectively, the charge and spin Luttinger parameters of the 1DEG, and the corresponding charge and spin velocities. The various bosonized fields satisfy the commutation relation $[\varphi_{\alpha}(x), \partial_x \theta_{\alpha}(x')] = i\delta(x - x')$, and similarly for $\tilde{\theta}_s, \tilde{\varphi}_s$. We neglect marginally irrelevant contributions to H_{Heis} .

For a *an* incommensurate filling n of the 1DEG, only “forward scattering” terms in the spin channel can couple the 1DEG and the spin chain. Up to irrelevant (backscattering) operators, the Kondo Hamiltonian density is $\mathcal{H}_K = \frac{J_K a}{8\pi} [(\partial_x \varphi_+)^2 - (\partial_x \varphi_-)^2] + \mathcal{H}_{\text{int}}$ [13] where $\theta_{\pm} = \frac{1}{\sqrt{2}}(\tilde{\theta}_s \pm \theta_s)$, $\varphi_{\pm} = \frac{1}{\sqrt{2}}(\tilde{\varphi}_s \pm \varphi_s)$, and $\mathcal{H}_{\text{int}} = \frac{\cos(\sqrt{4\pi}\theta_-)}{2(\pi a)^2} [\cos(\sqrt{4\pi}\varphi_+) + \cos(\sqrt{4\pi}\varphi_-)]$. (a is a microscopic cutoff.) Under renormalization, $\cos(\sqrt{4\pi}\theta_-) \cos(\sqrt{4\pi}\varphi_+)$ is marginally relevant [13], while $\cos(\sqrt{4\pi}\theta_-) \cos(\sqrt{4\pi}\varphi_-)$ is irrelevant, since it contains the dual fields θ_- and φ_- . The strong coupling phase has a spin gap, while the charge degree of freedom φ_c remains decoupled and gapless.

Correlations in the spin gapped phase: The form of the dominant (slowest decaying) correlations follows from the following considerations. A theorem by Yamanaka *et. al.* [26] guarantees the existence of a charge zero, momentum $2k_F^* = \pi n_{\text{tot}}$ gapless excitation, where n_{tot} is

the total electron density in the system (counting both the 1DEG and the spin chain). Here, $n_{\text{tot}} = n + \frac{1}{b}$, therefore $2k_F^* = 2k_F + \pi/b$. Let us denote the operator that creates these excitations $\hat{O}_{2k_F^*}$. Since there is a spin gap, $\hat{O}_{2k_F^*}$ is necessarily a spin singlet, *i.e.*, a CDW operator.

In addition, as long as there is no charge gap, the singlet “ η -pairing operator”[16, 20] $\hat{O}_\eta = \psi_{-\uparrow}\psi_{-\downarrow} = \frac{1}{2\pi a} \exp[i\sqrt{2\pi}(\theta_c - \phi_c)]$, also creates gapless excitations. ($\psi_{\pm,\sigma}$ annihilate right/left moving electrons with spin $\sigma = \uparrow, \downarrow$, respectively.) This operator has total momentum $-2k_F$ and charge $2e$. Therefore, the “PDW operator” $\hat{O}_{\text{PDW}} = \hat{O}_\eta \hat{O}_{2k_F^*}$ also creates gapless excitations. Adding the quantum numbers carried by \hat{O}_η and $\hat{O}_{2k_F^*}$, we see that \hat{O}_{PDW} carries charge $2e$ and momentum π/b . This guarantees the existence of quasi-long range PDW correlations in the spin gapped phase. As usual, the correlations of \hat{O}_{PDW} (as well as those of $\hat{O}_{2k_F^*}$) fall off with a non-universal exponent, which depends on K_c . The (zero momentum) Cooper pair operator is $\hat{O}_{SC} = \psi_{+\uparrow}\psi_{-\downarrow} = \frac{1}{2\pi a} e^{i\sqrt{2\pi}(\theta_c + \phi_s)}$. Its correlations are short ranged, since $\phi_s = (\phi_+ + \phi_-)/\sqrt{2}$; in the spin gapped phase the field θ_- is pinned, while its dual ϕ_- undergoes strong fluctuations, suppressing the correlations of \hat{O}_{SC} . Consequently, the leading superconducting correlations are for operators with non-zero momentum.

Generically, any singlet operator that carries charge $2e$ and momentum π/b is expected to couple to \hat{O}_{PDW} , and therefore to have quasi-long range correlations. For example, both ϕ_{PDW} and ϕ_c defined above have the correct quantum numbers, and therefore their correlations should fall off with the same exponent as that of \hat{O}_{PDW} . According to our numerical simulations, the spin gapped phase has strong PDW correlations, so it is best characterized by the ϕ_{PDW} order parameter. The results in Fig. 3 are fully consistent with the field theoretic analysis above. In particular, the density profile shows a large peak at $q = 2k_F^*$ which grows with system size, indicating slowly decaying fluctuations centered at that wavevector. The pairing correlations are strongly peaked at $q = \pi/b$, with a subdominant peak (which does not grow with L) at $q = 2k_F$, corresponding to the gapless η pairing mode.

Discussion: The correlations in the spin gapped phase of the 1D KHM are best described as a PDW phase, which is a (quasi-)condensate of non-zero center of mass momentum Cooper pairs. Locally, the correlations are strikingly similar to those of the PDW state recently proposed to describe the striped phase of $\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$, which intertwines spin, charge, and density orders. A study of a two-chain KHM found, instead, dominant uniform pairing correlations[27]. It remains an important question whether the PDW state survives in other multi-chain generalizations of the present model. Finally, the 1D KHM can be viewed as a variation of the three-band copper-oxide model[28], with strongly localized spins on the Cu sites and a 1DEG representing

doped holes on O sites. Therefore it seems plausible that such a model can exhibit a PDW phase as well. Whether it can be realized in the physically relevant parameter regime remains to be seen.

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Supplementary information

Throughout the paper, we have used various boundary perturbations (either pairing fields, Zeeman fields, or the boundary itself) to excite various sorts of order parameters. The decay of these order parameters into the bulk gives information on the leading response of the system. In order to verify that our results (in particular, the fact that the dominant pairing fluctuations are at a non-zero wavevector) are not induced by the external boundary perturbations, we have made the following additional checks:

1. We have varied the strength of the bond-centered boundary pair field, H_{pair} , in the range $\Delta = 0.1 - 0.5t$;
2. We tried to apply an on-site pair field on the first site, rather than a bond-centered pair field, in order to verify that the nature of the correlations is not sensitive to the form of the pair fields; and
3. We set $\Delta = 0$ and calculated the equal-time pair-pair correlation function.

In this Supplementary Information, we describe these results of these calculations. In all cases, the doping of the 1D electron gas was $n = 1.125$ particles per site, and the following parameters were used: $J_H/t = J_K/t = 2$.

Dependence on the boundary pair field strength

Fig. 5 shows the induced pair fields

$$\begin{aligned}\phi(j) &= \langle c_{j\uparrow}^\dagger c_{j\downarrow}^\dagger \rangle \\ \phi_B(j) &= \frac{1}{2} \langle c_{j\uparrow}^\dagger c_{j+1\downarrow}^\dagger - c_{j\downarrow}^\dagger c_{j+1\uparrow}^\dagger \rangle,\end{aligned}\quad (10)$$

in three calculations, in which a bond-centered pair field

$$H_{\text{pair}} = \Delta(c_{j\uparrow}^\dagger c_{j+1\downarrow}^\dagger - c_{j\downarrow}^\dagger c_{j+1\uparrow}^\dagger + H.c.) \quad (11)$$

was applied to the first bond with a varying strength: $\Delta/t = 0.1, 0.2, 0.5$. The system sizes were $L = 64$ in all calculations. The results are qualitatively similar to each other. In particular, the fact that the dominant response is at a non-zero wavevector $q = \pi/a$ does not depend on the value of Δ/t . Note that, between $\Delta/t = 0.1$ and 0.2, the response is roughly linear in the applied field. Between $\Delta/t = 0.2$ and 0.5, the response nearly saturates. In all cases, we found that the on-site order parameter $\phi(j)$ (not shown) decays very rapidly.

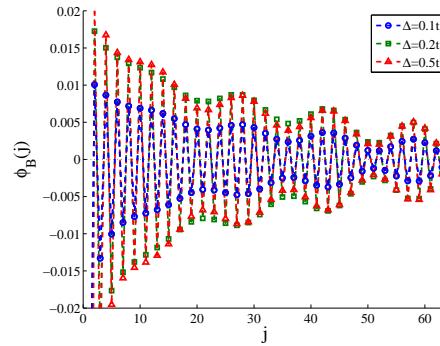


FIG. 5: Induced superconducting order parameters in $L = 64$ systems with bond-centered boundary pair fields of varying strength, as a function of position along the chain.

On-site boundary field

In Fig. 6, we plot $\phi(j)$ and $\phi_B(j)$ for an $L = 64$ system in which the following site-centered pair field was applied:

$$\tilde{H}_{\text{pair}} = \Delta c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger + H.c., \quad (12)$$

with $\Delta = 0.5t$. The results are very similar to the case of a bond-centered boundary pair field: the on-site order

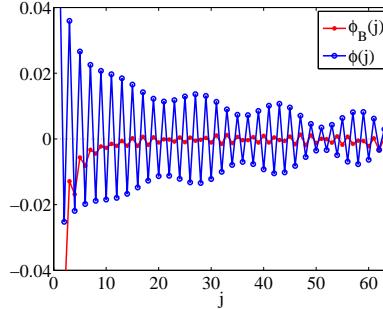


FIG. 6: Induced superconducting order parameters, ϕ and ϕ_B (see Eq. 10), in an $L = 64$ system with a site-centered boundary pair fields of strength $\Delta/t = 0.5$.

parameter $\phi(j)$ decays very rapidly, while a bond-centered order parameter $\phi_B(j)$ is induced. $\phi_B(j)$ oscillates at a wavevector $q = \pi/a$ and its amplitude decays slowly. This shows that the induced order parameter far away from the edges is not sensitive to the details of the edge fields.

Equal-time correlations

Finally, we calculate the pair-pair correlation function

$$C(x) = \langle \phi_B([L/2 - x/2]) \phi_B([L/2 + x/2]) \rangle \quad (13)$$

in an $L = 16$ system. $[.]$ represents rounding to the nearest integer from below. The results (Fig 7) clearly show that beyond the first few neighbors, $C(x)$ oscillates with a period of a , i.e. the dominant superconducting correlations are pair density wave correlations, in agreement with measurements of the response to edge fields.

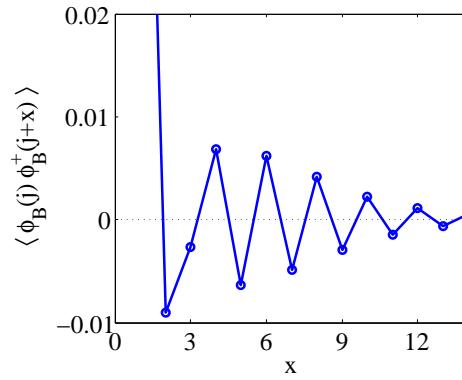


FIG. 7: The equal-time two-point superconducting correlation function (Eq. 13) as a function of distance x .